Machine Learning for Data Science (CS4786)
Lecture 8

Kernel PCA
&
Isomap

Kernel Trick

- We have have nice methods for linear dimensionality reduction
- Can we use this beyond the linear realm?

Kernel Trick

- Lift to higher dimensions (introduces non-linearity)
  - Using feature map $\phi(x)$
- Perform linear dimensionality reduction in this high dimensional space

Key Idea:

If an algorithm only depends on inner products, we can simply replace inner product in x space by inner product in $\phi(x)$ space

Can we write PCA so it only depends on inner products?

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$$\lambda_k W_k = \frac{1}{n}\left(\sum_{t=1}^{n} \mathbf{x}_t \mathbf{x}_t^\top\right) W_k = \frac{1}{n}\sum_{t=1}^{n} \left(\mathbf{x}_t^\top W_k\right)\mathbf{x}_t$$

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$$\begin{aligned}
\mathbf{y}_s[k] &= W_k^\top \mathbf{x}_s \\
&= \frac{1}{\lambda_k}\left(\frac{1}{n}\sum_{t=1}^{n}\mathbf{y}_t[k]\mathbf{x}_t\right)^\top \mathbf{x}_s \\
&= \frac{1}{n\lambda_k}\sum_{t=1}^{n}\mathbf{y}_t[k]\mathbf{x}_t^\top \mathbf{x}_s \\
&= \frac{1}{n\lambda_k}\sum_{t=1}^{n}\mathbf{y}_t[k]\tilde{K}_{s,t}
\end{aligned}$$

Where $\tilde{K}_{s,t} = \mathbf{x}_t^\top \mathbf{x}_s$ is the kernel matrix for centered data

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Hence $P_k = \mathbf{y}[k]/\sqrt{n\lambda_k}$ is an eigenvector of $\tilde{K}$ with eigen value $\gamma_k = n\lambda_k$

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$$\tilde{K}_{s,t} = \left(\mathbf{x}_t - \frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u\right)^{\top}\left(\mathbf{x}_s - \frac{1}{n}\sum_{u=1}^{n}\mathbf{x}_u\right)$$

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Rewriting PCA

- Equivalently, if Kern is the matrix ($\text{Kern}_{t,s} = x_t^\top x_s$),

$$\tilde{K} = \text{Kern} - \frac{(\mathbf{1}_{n\times n} \times \text{Kern})}{n} - \frac{(\text{Kern} \times \mathbf{1}_{n\times n})}{n} + \frac{(\mathbf{1}_{n\times n} \times \text{Kern} \times \mathbf{1}_{n\times n})}{n^2}$$

Kernel PCA

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1.

n Kern n $=$

$$\begin{bmatrix} k(x_1,x_1) & k(x_1,x_2) & \dots & k(x_1,x_n) \\ k(x_2,x_1) & k(x_2,x_2) & \dots & k(x_2,x_n) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ k(x_{n-1},x_1) & k(x_{n-1},x_2) & \dots & k(x_{n-1},x_n) \\ k(x_n,x_1) & k(x_n,x_2) & \dots & k(x_n,x_n) \end{bmatrix}$$

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2.

n $\tilde{K}$ n $= \text{Kern} - \frac{1}{n}(\mathbf{1}\ \text{Kern} + \text{Kern}\ \mathbf{1}) + \frac{1}{n^2}\mathbf{1}\ \text{Kern}\ \mathbf{1}$

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$$3.\left[\underset{K}{\overset{n}{P}},\gamma\right] = \mathrm{eigs}\left(\tilde{K}, K\right)$$

Kernel PCA

3. $\left[\underset{K}{P}, \gamma \right] = \text{eigs}\left(\tilde{K}, K \right)$

4. $Y = \underset{K}{\begin{bmatrix} P_1\sqrt{\gamma_1} & \cdots & P_K\sqrt{\gamma_K} \end{bmatrix}}$

Kernel Methods: A note

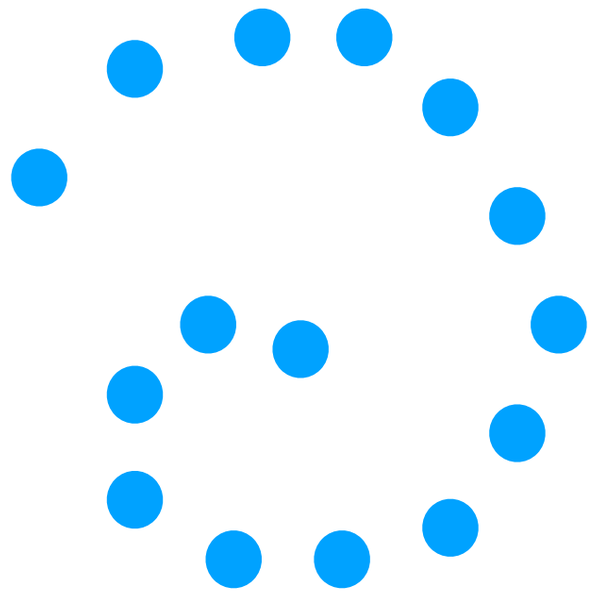
- We can “kernelize” CCA and many other linear dimensionality reduction methods.

- For any linear method, solution lies within linear span of data

- For typical linear methods y’s can be computed only based on inner products.

Manifold Based Dimensionality Reduction

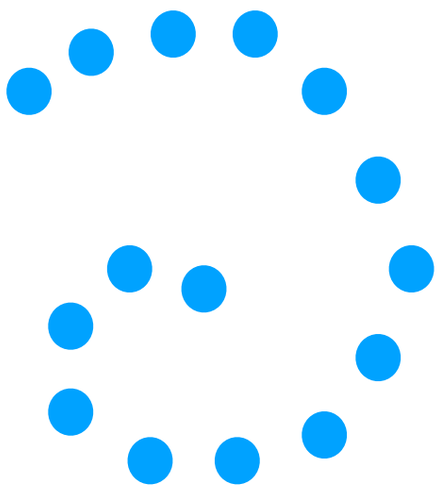
- Key Assumption: Points live on a low dimensional manifold
- Manifold: subspace that looks locally Euclidean
- Given data, can we uncover this manifold?



Can we unfold this?

Method I: Isomap

1. For every point, find its (k-) Nearest Neighbors



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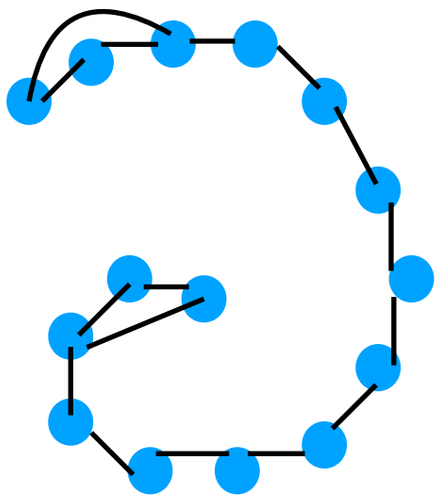

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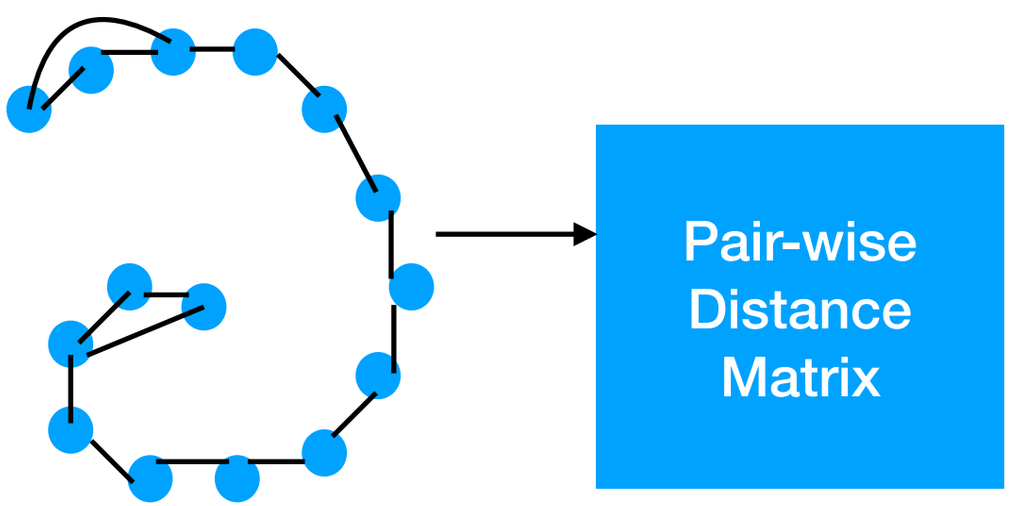

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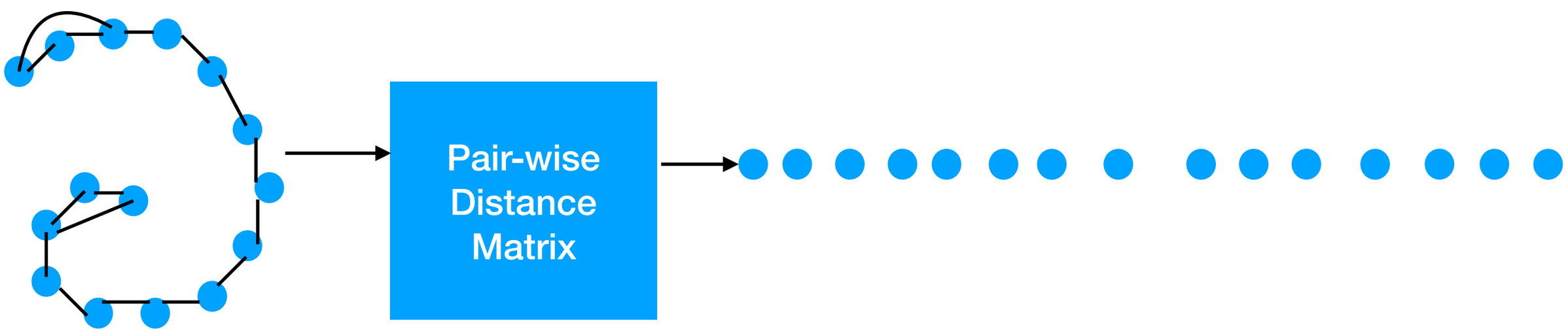

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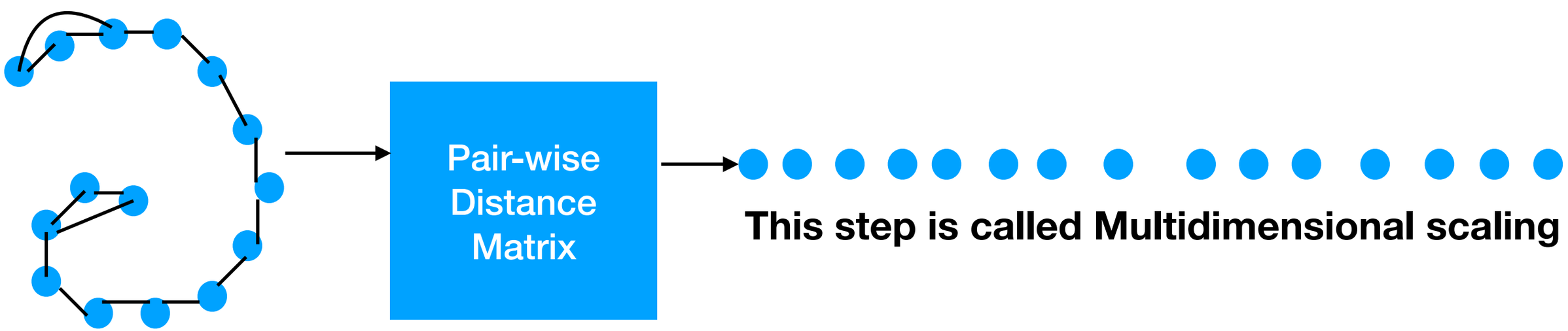

Isomap: Pitfalls

1. If we don't take enough nearest neighbors, then graph may not be connected

2. If we connect points too far away, points that should not be connected can get connected

3. There may not be a right number of nearest neighbors we should consider!

Demo